Connecting via Winsock to STN

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LOGINID:ssspta1623zct

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2		"Ask CAS" for self-help around the clock
NEWS 3	May 12	EXTEND option available in structure searching
NEWS 4	May 12	Polymer links for the POLYLINK command completed in REGISTRY
NEWS 5	May 27	New UPM (Update Code Maximum) field for more efficient patent SDIs in CAplus
NEWS 6	May 27	CAplus super roles and document types searchable in REGISTRY
NEWS 7	Jun 28	Additional enzyme-catalyzed reactions added to CASREACT
NEWS 8	Jun 28	ANTE, AQUALINE, BIOENG, CIVILENG, ENVIROENG, MECHENG, and WATER from CSA now available on STN(R)
NEWS 9	Jul 12	BEILSTEIN enhanced with new display and select options, resulting in a closer connection to BABS
NEWS 10	Jul 30	BEILSTEIN on STN workshop to be held August 24 in conjunction with the 228th ACS National Meeting
NEWS 11	AUG 02	IFIPAT/IFIUDB/IFICDB reloaded with new search and display fields
NEWS 12	AUG 02	CAplus and CA patent records enhanced with European and Japan Patent Office Classifications
NEWS 13	AUG 02	STN User Update to be held August 22 in conjunction with the 228th ACS National Meeting
NEWS 14	AUG 02	The Analysis Edition of STN Express with Discover! (Version 7.01 for Windows) now available
NEWS 15	AUG 04	Pricing for the Save Answers for SciFinder Wizard within STN Express with Discover! will change September 1, 2004
NEWS 16	AUG 27	BIOCOMMERCE: Changes and enhancements to content coverage
NEWS 17	AUG 27	BIOTECHABS/BIOTECHDS: Two new display fields added for legal status data from INPADOC
NEWS 18	SEP 01	INPADOC: New family current-awareness alert (SDI) available
NEWS 19	SEP 01	New pricing for the Save Answers for SciFinder Wizard within STN Express with Discover!
NEWS 20	SEP 01	New display format, HITSTR, available in WPIDS/WPINDEX/WPIX

NEWS EXPRESS	JULY 30 CURRENT WINDOWS VERSION IS V7.01, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004
NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS INTER	General Internet Information
NEWS LOGIN	Welcome Banner and News Items
NEWS PHONE	Direct Dial and Telecommunication Network Access to STN
NEWS WWW	CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

* * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 10:43:22 ON 08 SEP 2004

=> FILE REG

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 10:43:34 ON 08 SEP 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 7 SEP 2004 HIGHEST RN 741217-26-5
DICTIONARY FILE UPDATES: 7 SEP 2004 HIGHEST RN 741217-26-5

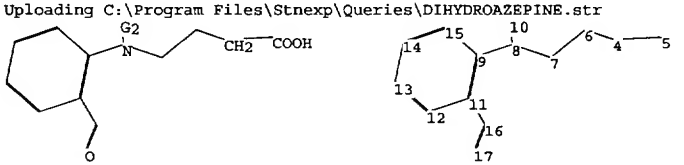
TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\DIHYDROAZEPINE.str



chain nodes :
4 5 10 16 17
ring nodes :
9 11 12 13 14 15
ring/chain nodes :
6 7 8
chain bonds :
4-5 4-6 6-7 7-8 8-9 8-10 11-16 16-17
ring bonds :
9-11 9-15 11-12 12-13 13-14 14-15
exact/norm bonds :
7-8 8-9 8-10 16-17
exact bonds :
4-5 4-6 6-7 11-16
normalized bonds :
9-11 9-15 11-12 12-13 13-14 14-15

G1:N,P,X,CF2,CF3,CCl2,CCl3,CBr2,CBr3,CI2,CI3,CN,NO2,Cy

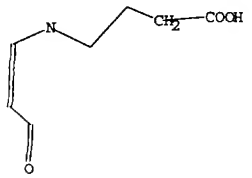
10/070329
UPDATED STN
SEARCH TRANSCRIPT

G2:C,S

Match level :
4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:Atom 12:Atom
13:Atom 14:Atom 15:Atom 16:CLASS 17:CLASS

L1 STRUCTURE UPLOADED

=> D L1
L1 HAS NO ANSWERS
L1 STR



G1 N,P,X,CF2,CF3,CCl2,CCl3,CBr2,CBr3,CI2,CI3,CN,NO2,Cy
G2 C,S

Structure attributes must be viewed using STN Express query preparation.

=> S L1
SAMPLE SEARCH INITIATED 10:43:54 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 23672 TO ITERATE

4.2% PROCESSED 1000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 464240 TO 482640
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> S L1 SSS FULL
FULL SEARCH INITIATED 10:44:10 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 474700 TO ITERATE

84.3% PROCESSED 400000 ITERATIONS 7 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.07

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 474700 TO 474700
PROJECTED ANSWERS: 7 TO 16

L3 7 SEA SSS FUL L1

=> FILE CAPLUS
COST IN U.S. DOLLARS SINCE FILE TOTAL

	ENTRY	SESSION
FULL ESTIMATED COST	155.42	155.63

FILE 'CAPLUS' ENTERED AT 10:44:26 ON 08 SEP 2004
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FILE COVERS 1907 - 8 Sep 2004 VOL 141 ISS 11
FILE LAST UPDATED: 7 Sep 2004 (20040907/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> S L3
L4 2 L3

=> D 1-2 IBIB ABS HITSTR

L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2004:331762 CAPLUS
DOCUMENT NUMBER: 140:339635
TITLE: Preparation of GABA analogs as prodrugs
INVENTOR(S): Gallop, Mark A.; Cundy, Kenneth C.; Zhou, Cindy X.; Qiu, Fayang G.; Yao, Fenmei; Xiang, Jia-Ning; Ollmann, Ian R.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 52 pp., Cont.-in-part of U.S. Ser. No. 171,485.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004077553	A1	20040422	US 2002-313825	20021206
US 2003176398	A1	20030918	US 2002-171485	20020611
US 2004006132	A1	20040108	US 2003-459242	20030610
WO 2003104184	A1	20031218	WO 2003-US18495	20030611
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
WO 2004052844	A1	20040624	WO 2003-US38703	20031205

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD

RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2001-297521P P 20010611
US 2001-298514P P 20010614
US 2002-366090P P 20020319
US 2002-171485 A2 20020611
US 2002-313825 A 20021206

OTHER SOURCE(S): MARPAT 140:339635

AB The invention provides prodrugs of GABA analogs and pharmaceutical compns. containing these prodrugs for treating or preventing common diseases and/or disorders. Compds. of formulas R1(X-CHR2CO)nNHCHR3CR4R5CHR6CO-Y-R7 [n = 0 or 1; X = O or an imino group; Y = O or S; R1 = (thio)acyl or phosphoryl groups, alkylthio, arylthio, etc.; R2-R7 = H, (cyclo)alkyl, aryl, etc.; CR4R5 = (un)substituted cyclo(hetero)alkyl, bridged cycloalkyl], R20R21C:(NCHR2CO)t(X-CHR2CO)uNHCHR3CR4R5CHR6CO-Y-R7 [t, u = 0 or 1; R20, R21 = groups similar to R4 and R5] , and R1(X-CHR2CO)nNRCHR3CR4R5CHR6CO-R [R2 = CR22R23O (to form a lactone), where R22, R23 are groups similar to R4 and R5] are claimed. Thus, 1-[[[[(pivaloyloxy)methoxy]carbonyl]amino]methyl]-1-cyclohexaneacetic acid (51) was prepared by acylation of gabapentin with p-nitrophenyl pivaloyloxymethyl carbonate (preparation given). In vitro Caco-2 cellular permeabilities of the prodrugs were determined, with compound 51 having Papp (apical to basolateral) and Papp (basolateral to apical) values of 1.06x10-4 and 1.25x10-5 cm/s, resp.

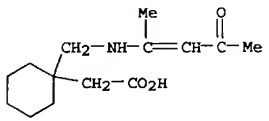
IT **478297-11-9P 478297-17-5P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of GABA analogs as prodrugs)

RN 478297-11-9 CAPLUS

CN Cyclohexaneacetic acid, 1-[[(1-methyl-3-oxo-1-butenyl)amino]methyl]-, compd. with piperidine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 478297-10-8
CMF C14 H23 N O3



CM 2

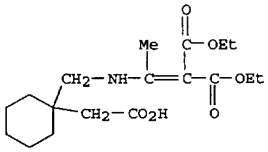
CRN 110-89-4
CMF C5 H11 N

RN 478297-17-5 CAPLUS

CN Propanedioic acid, [1-[[[1-(carboxymethyl)cyclohexyl]methyl]amino]ethylidene]-, 1,3-diethyl ester, compd. with piperidine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 478297-16-4
CMF C18 H29 N O6



CM 2

CRN 110-89-4
CMF C5 H11 N

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:964141 CAPLUS
DOCUMENT NUMBER: 138:24958
TITLE: Preparation of GABA analogs as prodrugs
INVENTOR(S): Gallop, Mark A.; Cundy, Kenneth C.; Zhou, Cindy X.; Yao, Fenmei; Xiang, Jia-Ning; Ollman, Ian R.; Qui, Fayang G.
PATENT ASSIGNEE(S): Xenoport, Inc., USA
SOURCE: PCT Int. Appl., 148 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002100347	A2	20021219	WO 2002-US18689	20020611
WO 2002100347	A3	20031016		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,

LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 2003083382	A1	20030501	US 2002-170127		20020611
EP 1404324	A2	20040407	EP 2002-744314		20020611

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

PRIORITY APPLN. INFO.:	US 2001-297521P	P	20010611
	US 2001-298514P	P	20010614
	US 2002-366090P	P	20020319
	WO 2002-US18689	W	20020611

OTHER SOURCE(S): MARPAT 138:24958

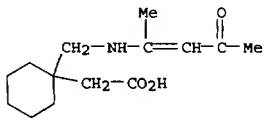
AB The invention provides prodrugs of GABA analogs and pharmaceutical compns. containing these prodrugs for treating or preventing common diseases and/or disorders. Compds. of formulas R1(X-CHR2CO)nNHCHR3CR4R5CHR6CO-Y-R7 [n = 0 or 1; X = O or an imino group; Y = O or S; R1 = (thio)acyl or phosphoryl groups, alkylthio, arylthio, etc.; R2-R7 = H, (cyclo)alkyl, aryl, etc.; CR4R5 = (un)substituted cyclo(hetero)alkyl, bridged cycloalkyl], R20R21C:(NCHR2CO)t(X-CHR2CO)uNHCHR3CR4R5CHR6CO-Y-R7 [t, u = 0 or 1; R20, R21 = groups similar to R4 and R5] , and R1(X-CHR2CO)nNRCHR3CR4R5CHR6CO-R [R2 = CR22R23O (to form a lactone), where R22, R23 are groups similar to R4 and R5] are claimed. Thus, 1-[[[[(pivaloyloxy)methoxy]carbonyl]amino]methyl]-1-cyclohexaneacetic acid (51) was prepared by acylation of gabapentin with p-nitrophenyl pivaloyloxymethyl carbonate (preparation given). In vitro Caco-2 cellular permeabilities of the prodrugs were determined, with compound 51 having Papp (apical to basolateral) and Papp (basolateral to apical) values of 1.06x10-4 and 1.25x10-5 cm/s, resp.

IT **478297-11-9P 478297-17-5P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of GABA analogs as prodrugs)

RN 478297-11-9 CAPLUS
CN Cyclohexaneacetic acid, 1-[[(1-methyl-3-oxo-1-butenyl)amino]methyl]-, compd. with piperidine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 478297-10-8
CMF C14 H23 N O3



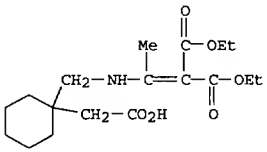
CM 2

CRN 110-89-4
CMF C5 H11 N

RN 478297-17-5 CAPLUS
CN Propanedioic acid, [1-[[[1-(carboxymethyl)cyclohexyl]methyl]amino]ethylidene]-, 1,3-diethyl ester, compd. with piperidine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 478297-16-4
CMF C18 H29 N O6



CM 2

CRN 110-89-4
CMF C5 H11 N

=> FILE REG

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	11.72	167.35
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-1.40	-1.40

FILE 'REGISTRY' ENTERED AT 10:47:42 ON 08 SEP 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 7 SEP 2004 HIGHEST RN 741217-26-5
DICTIONARY FILE UPDATES: 7 SEP 2004 HIGHEST RN 741217-26-5

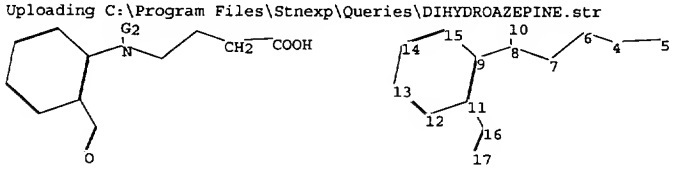
TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\DIHYDROAZEPINE.str



chain nodes :
4 5 10 16 17
ring nodes :
9 11 12 13 14 15
ring/chain nodes :
6 7 8
chain bonds :
4-5 4-6 6-7 7-8 8-9 8-10 11-16 16-17
ring bonds :
9-11 9-15 11-12 12-13 13-14 14-15
exact/norm bonds :
7-8 8-9 8-10 16-17
exact bonds :
4-5 4-6 6-7 11-16
normalized bonds :
9-11 9-15 11-12 12-13 13-14 14-15

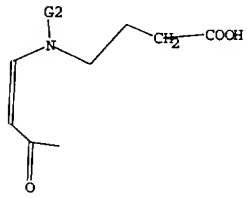
G1:N,P,X,CF2,CF3,CCl2,CCl3,CBr2,CBr3,CI2,CI3,CN,NO2,Cy

G2:C,S

Match level :
4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:Atom 12:Atom
13:Atom 14:Atom 15:Atom 16:CLASS 17:CLASS

L5 STRUCTURE UPLOADED

=> D L5
L5 HAS NO ANSWERS
L5 STR



G1 N,P,X,CF2,CF3,CCl2,CCl3,CBr2,CBr3,CI2,CI3,CN,NO2,Cy
G2 C,S

Structure attributes must be viewed using STN Express query preparation.

=> S L5
SAMPLE SEARCH INITIATED 10:48:39 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 405 TO ITERATE

100.0% PROCESSED 405 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 6893 TO 9307
PROJECTED ANSWERS: 0 TO 0

L6 0 SEA SSS SAM L5

=> S L5 SSS FULL
FULL SEARCH INITIATED 10:48:46 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 8040 TO ITERATE

100.0% PROCESSED 8040 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L7 0 SEA SSS FUL L5

=> FILE CAPLUS
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 157.10 324.45

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE ENTRY TOTAL SESSION
CA SUBSCRIBER PRICE 0.00 -1.40

FILE 'CAPLUS' ENTERED AT 10:50:41 ON 08 SEP 2004
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FILE COVERS 1907 - 8 Sep 2004 VOL 141 ISS 11
FILE LAST UPDATED: 7 Sep 2004 (20040907/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> S 2001:185710/AN
L8 1 2001:185710/AN

=> D

L8 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN
AN **2001:185710** CAPLUS
DN 134:222638
TI Process for the preparation of 2,3-dihydroazepine compounds
IN Ikemoto, Tomomi; Ito, Tatsuya; Nishiguchi, Atsuko; Tomimatsu, Kiminori
PA Takeda Chemical Industries, Ltd., Japan
SO PCT Int. Appl., 59 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001017947	A1	20010315	WO 2000-JP6012	20000905
	W: AE, AG, AL, AM, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CN, CR, CU, CZ, DM, DZ, EE, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LV, MA, MD, MG, MK, MN, MX, MZ, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	AU 2000068706	A5	20010410	AU 2000-68706	20000905
	EP 1211239	A1	20020605	EP 2000-956925	20000905
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
	JP 2001151741	A2	20010605	JP 2000-275003	20000906
PRAI	JP 1999-252334	A	19990906		
	WO 2000-JP6012	W	20000905		

OS CASREACT 134:222638; MARPAT 134:222638
RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> SEL RN
E1 THROUGH E46 ASSIGNED

=> FILE REG

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	3.84	328.29

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-1.40

FILE 'REGISTRY' ENTERED AT 10:52:01 ON 08 SEP 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 7 SEP 2004 HIGHEST RN 741217-26-5
DICTIONARY FILE UPDATES: 7 SEP 2004 HIGHEST RN 741217-26-5

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=> S E1-E46
1 106-94-5/BI
(106-94-5/RN)
1 123-38-6/BI
(123-38-6/RN)
1 135-02-4/BI
(135-02-4/RN)
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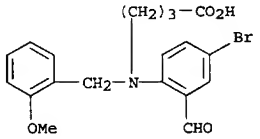
L9 46 (106-94-5/BI OR 123-38-6/BI OR 135-02-4/BI OR 251554-47-9/BI OR 2687-97-0/BI OR 313731-43-0/BI OR 313737-28-9/BI OR 329347-13-9/BI OR 329347-14-0/BI OR 329347-15-1/BI OR 329347-16-2/BI OR 329347-17-3/BI OR 329347-18-4/BI OR 329347-19-5/BI OR 329347-20-8/BI OR 329347-21-9/BI OR 329347-22-0/BI OR 329347-23-1/BI OR 329347-24-2/BI OR 329347-25-3/BI OR 329347-26-4/BI OR 329347-27-5/BI OR 329347-28-6/BI OR 329347-29-7/BI OR 329347-30-0/BI OR 329347-31-1/BI OR 329347-32-2/BI OR 329347-33-3/BI OR 329347-34-4/BI OR 329347-35-5/BI OR 3470-98-2/BI OR 3470-99-3/BI OR 3772-26-7/BI OR 39255-24-8/BI OR 446-52-6/BI OR 56-12-2/BI OR 616-45-5/BI OR 6361-21-3/BI OR 6837-24-7/BI OR 6976-17-6/BI OR 74-88-4/BI OR 74-96-4/BI OR 7439-95-4/BI OR 75-03-6/BI OR 77771-02-9/BI OR 93777-26-5/BI)

=> D 1-46

L9 ANSWER 1 OF 46 REGISTRY COPYRIGHT 2004 ACS on STN

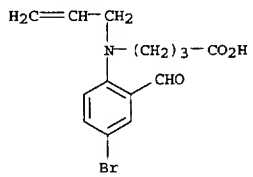
RN **329347-35-5** REGISTRY
CN Butanoic acid, 4-[(4-bromo-2-formylphenyl)[(2-methoxyphenyl)methyl]amino]- (9CI) (CA INDEX NAME)
MF C19 H20 Br N O4
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

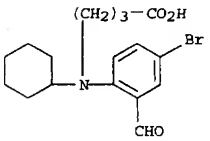
L9 ANSWER 2 OF 46 REGISTRY COPYRIGHT 2004 ACS on STN
RN **329347-34-4** REGISTRY
CN Butanoic acid, 4-[(4-bromo-2-formylphenyl)-2-propenylamino]- (9CI) (CA INDEX NAME)
MF C14 H16 Br N O3
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

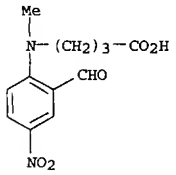
L9 ANSWER 3 OF 46 REGISTRY COPYRIGHT 2004 ACS on STN
RN **329347-33-3** REGISTRY
CN Butanoic acid, 4-[(4-bromo-2-formylphenyl)cyclohexylamino]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H22 Br N O3
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

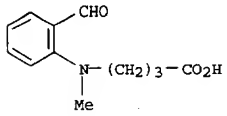
L9 ANSWER 4 OF 46 REGISTRY COPYRIGHT 2004 ACS on STN
RN **329347-32-2** REGISTRY
CN Butanoic acid, 4-[(2-formyl-4-nitrophenyl)methylamino]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C12 H14 N2 O5
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L9 ANSWER 5 OF 46 REGISTRY COPYRIGHT 2004 ACS on STN
RN **329347-31-1** REGISTRY
CN Butanoic acid, 4-[(2-formylphenyl)methylamino]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C12 H15 N O3
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)



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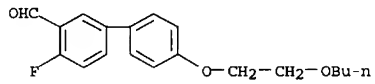
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

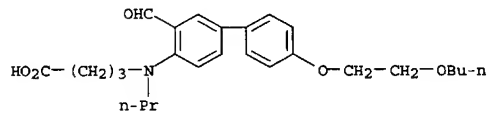
L9 ANSWER 6 OF 46 REGISTRY COPYRIGHT 2004 ACS on STN
RN **329347-30-0** REGISTRY
CN [1,1'-Biphenyl]-3-carboxaldehyde, 4'-(2-butoxyethoxy)-4-fluoro- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H21 F O3
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

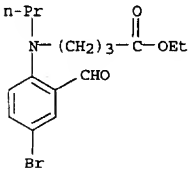
L9 ANSWER 7 OF 46 REGISTRY COPYRIGHT 2004 ACS on STN
RN **329347-29-7** REGISTRY
CN Butanoic acid, 4-[[4'-(2-butoxyethoxy)-3-formyl[1,1'-biphenyl]-4-yl]propylamino]- (9CI) (CA INDEX NAME)
MF C26 H35 N O5
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L9 ANSWER 8 OF 46 REGISTRY COPYRIGHT 2004 ACS on STN
RN **329347-28-6** REGISTRY
CN Butanoic acid, 4-[(4-bromo-2-formylphenyl)propylamino]-, ethyl ester (9CI) (CA INDEX NAME)
MF C16 H22 Br N O3
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)



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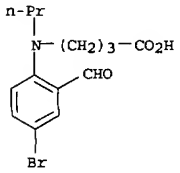
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

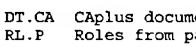
L9 ANSWER 9 OF 46 REGISTRY COPYRIGHT 2004 ACS on STN
RN **329347-27-5** REGISTRY
CN Butanoic acid, 4-[(4-bromo-2-formylphenyl)propylamino]- (9CI) (CA INDEX NAME)
MF C14 H18 Br N O3
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

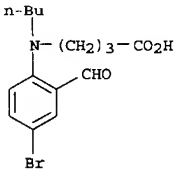
L9 ANSWER 10 OF 46 REGISTRY COPYRIGHT 2004 ACS on STN
RN **329347-26-4** REGISTRY
CN Butanoic acid, 4-(propylamino)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C7 H15 N O2
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

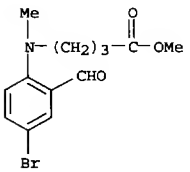
L9 ANSWER 11 OF 46 REGISTRY COPYRIGHT 2004 ACS on STN
RN **329347-25-3** REGISTRY
CN Butanoic acid, 4-[(4-bromo-2-formylphenyl)butylamino]- (9CI) (CA INDEX NAME)
MF C15 H20 Br N O3
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

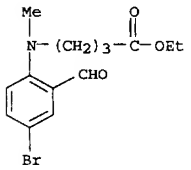
L9 ANSWER 12 OF 46 REGISTRY COPYRIGHT 2004 ACS on STN
RN **329347-24-2** REGISTRY
CN Butanoic acid, 4-[(4-bromo-2-formylphenyl)methylamino]-, methyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C13 H16 Br N O3
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

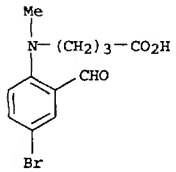
L9 ANSWER 13 OF 46 REGISTRY COPYRIGHT 2004 ACS on STN
RN **329347-23-1** REGISTRY
CN Butanoic acid, 4-[(4-bromo-2-formylphenyl)methylamino]-, ethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C14 H18 Br N O3
SR CA
LC STN Files: CA, CAPLUS, CASREACT
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L9 ANSWER 14 OF 46 REGISTRY COPYRIGHT 2004 ACS on STN
RN **329347-22-0** REGISTRY
CN Butanoic acid, 4-[(4-bromo-2-formylphenyl)methylamino]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C12 H14 Br N O3
SR CA
LC STN Files: CA, CAPLUS, CASREACT
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)

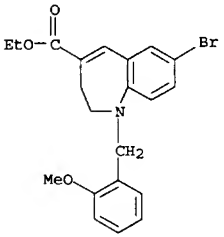


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

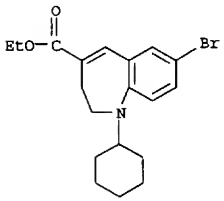
L9 ANSWER 15 OF 46 REGISTRY COPYRIGHT 2004 ACS on STN
RN **329347-21-9** REGISTRY
CN 1H-1-Benzazepine-4-carboxylic acid, 7-bromo-2,3-dihydro-1-[(2-methoxyphenyl)methyl]-, ethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C21 H22 Br N O3
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L9 ANSWER 16 OF 46 REGISTRY COPYRIGHT 2004 ACS on STN
RN **329347-20-8** REGISTRY
CN 1H-1-Benzazepine-4-carboxylic acid, 7-bromo-1-cyclohexyl-2,3-dihydro-, ethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H24 Br N O2
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation)

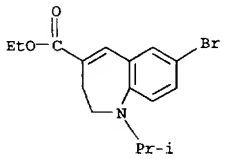


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

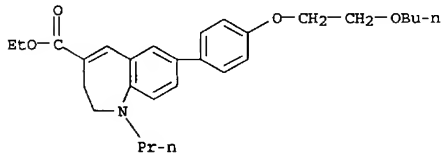
L9 ANSWER 17 OF 46 REGISTRY COPYRIGHT 2004 ACS on STN
RN **329347-19-5** REGISTRY
CN 1H-1-Benzazepine-4-carboxylic acid, 7-bromo-2,3-dihydro-1-(1-methylethyl)-, ethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C16 H20 Br N O2
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

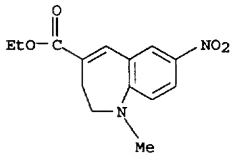
L9 ANSWER 18 OF 46 REGISTRY COPYRIGHT 2004 ACS on STN
RN **329347-18-4** REGISTRY
CN 1H-1-Benzazepine-4-carboxylic acid, 7-[4-(2-butoxyethoxy)phenyl]-2,3-dihydro-1-propyl-, ethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C28 H37 N O4
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

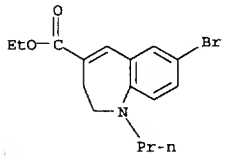
L9 ANSWER 19 OF 46 REGISTRY COPYRIGHT 2004 ACS on STN
RN **329347-17-3** REGISTRY
CN 1H-1-Benzazepine-4-carboxylic acid, 2,3-dihydro-1-methyl-7-nitro-, ethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C14 H16 N2 O4
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

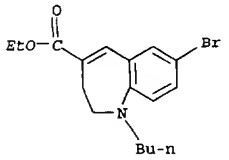
L9 ANSWER 20 OF 46 REGISTRY COPYRIGHT 2004 ACS on STN
RN **329347-16-2** REGISTRY
CN 1H-1-Benzazepine-4-carboxylic acid, 7-bromo-2,3-dihydro-1-propyl-, ethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C16 H20 Br N O2
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

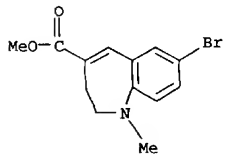
L9 ANSWER 21 OF 46 REGISTRY COPYRIGHT 2004 ACS on STN
RN **329347-15-1** REGISTRY
CN 1H-1-Benzazepine-4-carboxylic acid, 7-bromo-1-butyl-2,3-dihydro-, ethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H22 Br N O2
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

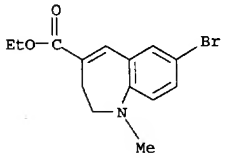
L9 ANSWER 22 OF 46 REGISTRY COPYRIGHT 2004 ACS on STN
RN **329347-14-0** REGISTRY
CN 1H-1-Benzazepine-4-carboxylic acid, 7-bromo-2,3-dihydro-1-methyl-, methyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C13 H14 Br N O2
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

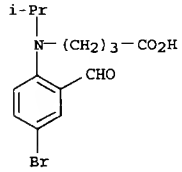
L9 ANSWER 23 OF 46 REGISTRY COPYRIGHT 2004 ACS on STN
RN **329347-13-9** REGISTRY
CN 1H-1-Benzazepine-4-carboxylic acid, 7-bromo-2,3-dihydro-1-methyl-, ethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C14 H16 Br N O2
SR CA
LC STN Files: CA, CAPLUS, CASREACT
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

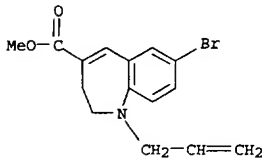
L9 ANSWER 24 OF 46 REGISTRY COPYRIGHT 2004 ACS on STN
RN **313737-28-9** REGISTRY
CN Butanoic acid, 4-[(4-bromo-2-formylphenyl)(1-methylethyl)amino]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C14 H18 Br N O3
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

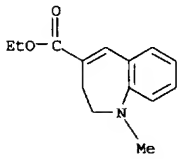
L9 ANSWER 25 OF 46 REGISTRY COPYRIGHT 2004 ACS on STN
RN **313731-43-0** REGISTRY
CN 1H-1-Benzazepine-4-carboxylic acid, 7-bromo-2,3-dihydro-1-(2-propenyl)-, methyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C15 H16 Br N O2
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

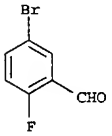
L9 ANSWER 26 OF 46 REGISTRY COPYRIGHT 2004 ACS on STN
RN **251554-47-9** REGISTRY
CN 1H-1-Benzazepine-4-carboxylic acid, 2,3-dihydro-1-methyl-, ethyl ester (9CI) (CA INDEX NAME)
OTHER NAMES:
CN Ethyl 1-methyl-2,3-dihydro-1H-benz[b]azepine-4-carboxylate
FS 3D CONCORD
MF C14 H17 N O2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

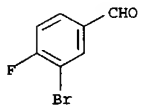
L9 ANSWER 27 OF 46 REGISTRY COPYRIGHT 2004 ACS on STN
RN **93777-26-5** REGISTRY
CN Benzaldehyde, 5-bromo-2-fluoro- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 3-Bromo-6-fluorobenzaldehyde
CN 5-Bromo-2-fluorobenzaldehyde
FS 3D CONCORD
MF C7 H4 Br F O
SR European Union (EU)
LC STN Files: CA, CAPLUS, CASREACT, CHEMCATS, CHEMLIST, CSCHEM, TOXCENTER, USPAT2, USPATFULL
Other Sources: EINECS**
(**Enter CHEMLIST File for up-to-date regulatory information)
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)
RL.NP Roles from non-patents: RACT (Reactant or reagent)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

63 REFERENCES IN FILE CA (1907 TO DATE)
64 REFERENCES IN FILE CAPLUS (1907 TO DATE)

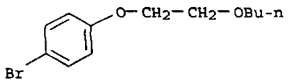
L9 ANSWER 28 OF 46 REGISTRY COPYRIGHT 2004 ACS on STN
RN **77771-02-9** REGISTRY
CN Benzaldehyde, 3-bromo-4-fluoro- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 3-Bromo-4-fluorobenzaldehyde
CN 4-Fluoro-3-bromobenzaldehyde
FS 3D CONCORD
MF C7 H4 Br F O
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, MSDS-OHS, SYNTHLINE, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: EINECS**, NDSL**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)
RL.NP Roles from non-patents: PREP (Preparation); PROC (Process); RACT (Reactant or reagent)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

108 REFERENCES IN FILE CA (1907 TO DATE)
108 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L9 ANSWER 29 OF 46 REGISTRY COPYRIGHT 2004 ACS on STN
RN **39255-24-8** REGISTRY
CN Benzene, 1-bromo-4-(2-butoxyethoxy)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN p-Bromobutoxyethoxybenzene
FS 3D CONCORD
MF C12 H17 Br O2
LC STN Files: CA, CAPLUS, USPATFULL
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)
RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

6 REFERENCES IN FILE CA (1907 TO DATE)
6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

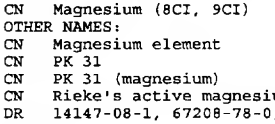
L9 ANSWER 30 OF 46 REGISTRY COPYRIGHT 2004 ACS on STN
RN **7439-95-4** REGISTRY
CN Magnesium (8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN Magnesium element
CN PK 31
CN PK 31 (magnesium)
CN Rieke's active magnesium
DR 14147-08-1, 67208-78-0, 199281-20-4, 298688-48-9
MF Mg
CI COM
LC STN Files: ANABSTR, AQUIRE, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CABA, CANCERLIT, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, CSNB, DDFU, DETHERM*, DRUGU, EMBASE, ENCOMPLIT, ENCOMPLIT2, ENCOMPPAT, ENCOMPPAT2, HSDB*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*, MSDS-OHS, NAPRALERT, NIOSHTIC, RTECS*, TOXCENTER, ULIDAT, USPAT2, USPATFULL, VETU, VTB
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)
DT.CA CAplus document type: Book; Conference; Dissertation; Journal; Patent; Preprint; Report
RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study); CMBI (Combinatorial study); FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)
RLD.P Roles for non-specific derivatives from patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)
RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); CMBI (Combinatorial study); FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)
RLD.NP Roles for non-specific derivatives from non-patents: ANST (Analytical study); BIOL (Biological study); CMBI (Combinatorial study); FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

199252 REFERENCES IN FILE CA (1907 TO DATE)
6799 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

199455 REFERENCES IN FILE CAPLUS (1907 TO DATE)

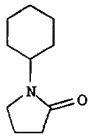
L9 ANSWER 31 OF 46 REGISTRY COPYRIGHT 2004 ACS on STN
RN **6976-17-6** REGISTRY
CN Butanoic acid, 4-(methylamino)-, hydrochloride (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 4-(Methylamino)butanoic acid hydrochloride
CN 4-(Methylamino)butyric acid hydrochloride
MF C5 H11 N O2 . Cl H
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, CHEMCATS, CSCHEM, MSDS-OHS, PS, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: RACT (Reactant or reagent)
RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)
CRN (1119-48-8)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

28 REFERENCES IN FILE CA (1907 TO DATE)
28 REFERENCES IN FILE CAPLUS (1907 TO DATE)

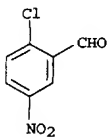
L9 ANSWER 32 OF 46 REGISTRY COPYRIGHT 2004 ACS on STN
RN **6837-24-7** REGISTRY
CN 2-Pyrrolidinone, 1-cyclohexyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN 1-Cyclohexyl-2-pyrrolidinone
CN 1-Cyclohexyl-2-pyrrolidone
CN N-Cyclohexyl-2-pyrrolidinone
CN N-Cyclohexyl-2-pyrrolidone
CN N-Cyclohexylpyrrolidinone
CN N-Cyclohexylpyrrolidone
FS 3D CONCORD
MF C10 H17 N O
CI COM
LC STN Files: BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, CSNB, DETHERM*, IFICDB, IFIPAT, IFIUDB, MEDLINE, MSDS-OHS, NIOSHTIC, PROMT, RTECS*, SPECINFO, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)
Other Sources: EINECS**, NDSL**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)
DT.CA CAplus document type: Conference; Journal; Patent; Report
RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study); MSC (Miscellaneous); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)
RLD.P Roles for non-specific derivatives from patents: PROC (Process); USES (Uses)
RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

264 REFERENCES IN FILE CA (1907 TO DATE)
4 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
264 REFERENCES IN FILE CAPLUS (1907 TO DATE)
5 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L9 ANSWER 33 OF 46 REGISTRY COPYRIGHT 2004 ACS on STN
RN **6361-21-3** REGISTRY
CN Benzaldehyde, 2-chloro-5-nitro- (6CI, 8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN 2-Chloro-5-nitrobenzaldehyde
CN 3-Nitro-6-chlorobenzaldehyde
CN 5-Nitro-2-chlorobenzaldehyde
CN 6-Chloro-3-nitrobenzaldehyde
CN NSC 129753
FS 3D CONCORD
MF C7 H4 Cl N O3
CI COM
LC STN Files: AQUIRE, BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM, HODOC*, IFICDB, IFIPAT, IFIUDB, RTECS*, SPECINFO, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: EINECS**, NDSL**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)
DT.CA CAplus document type: Conference; Journal; Patent
RL.P Roles from patents: PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)
RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); CMBI (Combinatorial study); FORM (Formation, nonpreparative); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); NORL (No role in record)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

259 REFERENCES IN FILE CA (1907 TO DATE)
259 REFERENCES IN FILE CAPLUS (1907 TO DATE)
3 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L9 ANSWER 34 OF 46 REGISTRY COPYRIGHT 2004 ACS on STN
RN **3772-26-7** REGISTRY
CN 2-Pyrrolidinone, 1-(1-methylethyl)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Pyrrolidinone, 1-isopropyl- (6CI, 7CI, 8CI)
OTHER NAMES:
CN 1-Isopropyl-2-pyrrolidinone
CN N-Isopropyl-2-pyrrolidinone
CN N-Isopropyl-2-pyrrolidone
CN N-Isopropylbutyrolactam
CN N-Isopropylpyrrolidinone
FS 3D CONCORD
MF C7 H13 N O
CI COM
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, HODOC*, IFICDB, IFIPAT, IFIUDB, RTECS*, SPECINFO, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)
Other Sources: EINECS**, NDSL**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)
RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)
RLD.NP Roles for non-specific derivatives from non-patents: PRP (Properties).

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

76 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
76 REFERENCES IN FILE CAPLUS (1907 TO DATE)
6 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L9 ANSWER 35 OF 46 REGISTRY COPYRIGHT 2004 ACS on STN
RN **3470-99-3** REGISTRY
CN 2-Pyrrolidinone, 1-propyl- (7CI, 8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN 1-Propyl-2-pyrrolidinone
CN 1-Propyl-2-pyrrolidone
CN 1-Propylazacyclopentan-2-one
CN N-Propyl-2-pyrrolidinone
CN N-Propyl-2-pyrrolidone
CN N-Propylpyrrolidone
FS 3D CONCORD
MF C7 H13 N O
CI COM
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, IFICDB, IFIPAT, IFIUDB, SPECINFO, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); PROC

(Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)
RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); NORL (No role in record)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

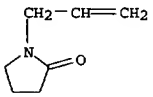
64 REFERENCES IN FILE CA (1907 TO DATE)
65 REFERENCES IN FILE CAPLUS (1907 TO DATE)
2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L9 ANSWER 36 OF 46 REGISTRY COPYRIGHT 2004 ACS on STN
RN **3470-98-2** REGISTRY
CN 2-Pyrrolidinone, 1-butyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN 1-Butyl-2-pyrrolidinone
CN 1-Butyl-2-pyrrolidone
CN N-Butyl-2-pyrrolidinone
CN N-Butyl-2-pyrrolidone
CN N-Butylbutyrolactam
CN N-Butylpyrrolidinone
CN N-Butylpyrrolidone
FS 3D CONCORD
MF C8 H15 N O
CI COM
LC STN Files: ANABSTR, BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM, DETHERM*, IFICDB, IFIPAT, IFIUDB, IPA, RTECS*, SPECINFO, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: EINECS**
(**Enter CHEMLIST File for up-to-date regulatory information)
DT.CA CAplus document type: Conference; Journal; Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)
RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

116 REFERENCES IN FILE CA (1907 TO DATE)
116 REFERENCES IN FILE CAPLUS (1907 TO DATE)
6 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L9 ANSWER 37 OF 46 REGISTRY COPYRIGHT 2004 ACS on STN
RN **2687-97-0** REGISTRY
CN 2-Pyrrolidinone, 1-(2-propenyl)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Pyrrolidinone, 1-allyl- (6CI, 7CI, 8CI)
OTHER NAMES:
CN 1-Allyl-2-oxopyrrolidine
CN 1-Allyl-2-pyrrolidinone
CN N-Allyl-2-pyrrolidinone
CN N-Allyl-2-pyrrolidone
CN N-Allylpyrrolidone
CN NSC 14674
FS 3D CONCORD
MF C7 H11 N O
CI COM
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, IFICDB, IFIPAT, IFIUDB, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: EINECS**
(**Enter CHEMLIST File for up-to-date regulatory information)
DT.CA CAplus document type: Conference; Journal; Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
RLD.P Roles for non-specific derivatives from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)
RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation); PRP (Properties); RACT (Reactant or reagent); NORL (No role in record)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

47 REFERENCES IN FILE CA (1907 TO DATE)
11 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
48 REFERENCES IN FILE CAPLUS (1907 TO DATE)
2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

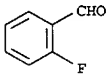
L9 ANSWER 38 OF 46 REGISTRY COPYRIGHT 2004 ACS on STN
RN **616-45-5** REGISTRY
CN 2-Pyrrolidinone (8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN α-Pyrrolidinone
CN α-Pyrrolidone
CN γ-Aminobutyric acid lactam
CN γ-Aminobutyric lactam
CN γ-Aminobutyrolactam
CN γ-Butyrolactam
CN 2-Oxopyrrolidine
CN 2-Pyrol
CN 2-Pyrrolidone
CN 2-Tetrahydropyrrolone
CN 4-Aminobutyric acid lactam
CN Azacyclopentan-2-one
CN Butanoic acid, 4-amino-, lactam

CN Butyrolactam
CN NSC 4593
CN NSC 8413
CN Pyrrolidone
FS 3D CONCORD
MF C4 H7 N O
CI COM
LC STN Files: AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CHEMSAFE, CIN, CSCHEM, DDFU, DETHERM*, DIPPR*, DRUGU, EMBASE, ENCOMPLIT, ENCOMPLIT2, ENCOMPPAT, ENCOMPPAT2, GMELIN*, HODOC*, HSDB*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*, MSDS-OHS, NAPRALERT, NIOSHTIC, PDLCOM*, PIRA, PROMT, PS, RTECS*, SPECINFO, SYNTHLINE, TOXCENTER, TULSA, USPAT2, USPATFULL, VTB
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)
DT.CA CAplus document type: Conference; Dissertation; Journal; Patent; Preprint; Report
RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); MSC (Miscellaneous); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)
RLD.P Roles for non-specific derivatives from patents: ANST (Analytical study); BIOL (Biological study); MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)
RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)
RLD.NP Roles for non-specific derivatives from non-patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); MSC (Miscellaneous); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3843 REFERENCES IN FILE CA (1907 TO DATE)
377 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
3850 REFERENCES IN FILE CAPLUS (1907 TO DATE)
58 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L9 ANSWER 39 OF 46 REGISTRY COPYRIGHT 2004 ACS on STN
RN **446-52-6** REGISTRY
CN Benzaldehyde, 2-fluoro- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Benzaldehyde, o-fluoro- (6CI, 7CI, 8CI)
OTHER NAMES:
CN 2-Fluorobenzaldehyde
CN NSC 66829
CN o-Fluorobenzaldehyde
FS 3D CONCORD
MF C7 H5 F O
CI COM
LC STN Files: ANABSTR, BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM, GMELIN*, HODOC*, IFICDB, IFIPAT, IFIUDB, PS, RTECS*, SPECINFO, SYNTHLINE, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: EINECS**
(**Enter CHEMLIST File for up-to-date regulatory information)
DT.CA CAplus document type: Conference; Journal; Patent; Report
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)
RLD.P Roles for non-specific derivatives from patents: USES (Uses)
RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); CMBI (Combinatorial study); FORM (Formation, nonpreparative); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)

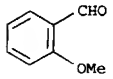


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1106 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
1111 REFERENCES IN FILE CAPLUS (1907 TO DATE)
15 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L9 ANSWER 40 OF 46 REGISTRY COPYRIGHT 2004 ACS on STN
RN **135-02-4** REGISTRY
CN Benzaldehyde, 2-methoxy- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Benzaldehyde, o-methoxy- (3CI)
CN o-Anisaldehyde (8CI)
OTHER NAMES:
CN 2-Anisaldehyde
CN 2-Methoxybenzaldehyde
CN 2-Methoxybenzenecarboxaldehyde
CN 2-Methoxyphenylformaldehyde
CN 6-Methoxybenzaldehyde
CN NC 064
CN NSC 58960
CN o-Formylanisole
CN o-Methoxybenzaldehyde
CN Salicylaldehyde methyl ether
FS 3D CONCORD
MF C8 H8 O2
CI COM
LC STN Files: AGRICOLA, ANABSTR, BEILSTEIN*, BIOBUSINESS, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM, DETHERM*, GMELIN*, HODOC*, HSDB*, IFICDB, IFIPAT, IFIUDB, MSDS-OHS, NAPRALERT, PROMT, RTECS*, SPECINFO, SYNTHLINE, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)
DT.CA CAplus document type: Conference; Journal; Patent; Report
RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)
RLD.P Roles for non-specific derivatives from patents: PREP (Preparation); USES (Uses)

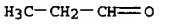
RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); CMBI (Combinatorial study); FORM (Formation, nonpreparative); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)
RLD.NP Roles for non-specific derivatives from non-patents: ANST (Analytical study); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2923 REFERENCES IN FILE CA (1907 TO DATE)
4 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
2931 REFERENCES IN FILE CAPLUS (1907 TO DATE)
7 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L9 ANSWER 41 OF 46 REGISTRY COPYRIGHT 2004 ACS on STN
RN **123-38-6** REGISTRY
CN Propanal (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Propionaldehyde (7CI, 8CI)
OTHER NAMES:
CN 1-Propanal
CN 1-Propanone
CN Ethylcarboxaldehyde
CN Methylacetaldehyde
CN n-Propanal
CN n-Propionaldehyde
CN NSC 6493
CN Propaldehyde
CN Propanaldehyde
CN Propional
CN Propionic aldehyde
CN Propylaldehyde
CN Propylic aldehyde
FS 3D CONCORD
MF C3 H6 O
CI COM
LC STN Files: AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CHEMSAFE, CIN, CSCHEM, CSNB, DDFU, DETHERM*, DIPPR*, DRUGU, EMBASE, ENCOMPLIT, ENCOMPLIT2, ENCOMPPAT, ENCOMPPAT2, GMELIN*, HODOC*, HSDB*, IFICDB, IFIPAT, IFIUDB, MEDLINE, MRCK*, MSDS-OHS, NAPRALERT, NIOSHTIC, PDLCOM*, PIRA, PROMT, PS, RTECS*, SPECINFO, SYNTHLINE, TOXCENTER, TULSA, ULIDAT, USPAT2, USPATFULL, VTB
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)
DT.CA CAplus document type: Book; Conference; Dissertation; Journal; Patent; Report
RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study); CMBI (Combinatorial study); FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)
RLD.P Roles for non-specific derivatives from patents: BIOL (Biological study); PREP (Preparation); PROC (Process); PRP (Properties); USES (Uses)
RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); CMBI (Combinatorial study); FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)
RLD.NP Roles for non-specific derivatives from non-patents: ANST (Analytical study); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

11425 REFERENCES IN FILE CA (1907 TO DATE)
101 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
11443 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L9 ANSWER 42 OF 46 REGISTRY COPYRIGHT 2004 ACS on STN
RN **106-94-5** REGISTRY
CN Propane, 1-bromo- (8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN 1-Bromopropane
CN 1-Propyl bromide
CN Ascusol MC
CN Leksol
CN n-Propyl bromide
CN Propyl bromide
FS 3D CONCORD
MF C3 H7 Br
CI COM
LC STN Files: ANABSTR, AQUIRE, BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CHEMSAFE, CIN, CSCHEM, CSNB, DETHERM*, DIPPR*, EMBASE, GMELIN*, HODOC*, HSDB*, IFICDB, IFIPAT, IFIUDB, MEDLINE, MRCK*, MSDS-OHS, NAPRALERT, NIOSHTIC, PIRA, PROMT, PS, RTECS*, SPECINFO, SYNTHLINE, TOXCENTER, USPAT2, USPATFULL, VTB
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)
DT.CA CAplus document type: Conference; Dissertation; Journal; Patent; Preprint; Report
RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study); MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)
RLD.P Roles for non-specific derivatives from patents: BIOL (Biological study); MSC (Miscellaneous); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)
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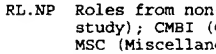
RLD.NP Roles for non-specific derivatives from non-patents: PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3902 REFERENCES IN FILE CA (1907 TO DATE)
42 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
3905 REFERENCES IN FILE CAPLUS (1907 TO DATE)
5 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L9 ANSWER 43 OF 46 REGISTRY COPYRIGHT 2004 ACS on STN
RN **75-03-6** REGISTRY
CN Ethane, iodo- (8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN Ethyl iodide
CN Hydriodic ether
CN Iodoethane
CN Monoiodoethane
CN NSC 8825
FS 3D CONCORD
MF C2 H5 I
CI COM
LC STN Files: AGRICOLA, ANABSTR, BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, CSNB, DETHERM*, DIPPR*, EMBASE, ENCOMPLIT, ENCOMPLIT2, ENCOMPPAT, ENCOMPPAT2, GMELIN*, HODOC*, IFICDB, IFIPAT, IFIUDB, MEDLINE, MRCK*, MSDS-OHS, NAPRALERT, NIOSHTIC, PIRA, PROMT, PS, RTECS*, SPECINFO, TOXCENTER, USPAT2, USPATFULL, VTB
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)
DT.CA CAplus document type: Conference; Dissertation; Journal; Patent; Preprint; Report
RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)
RLD.P Roles for non-specific derivatives from patents: BIOL (Biological study); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)
RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); CMBI (Combinatorial study); FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)
RLD.NP Roles for non-specific derivatives from non-patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

6442 REFERENCES IN FILE CA (1907 TO DATE)
68 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
6450 REFERENCES IN FILE CAPLUS (1907 TO DATE)
6 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L9 ANSWER 44 OF 46 REGISTRY COPYRIGHT 2004 ACS on STN
RN **74-96-4** REGISTRY
CN Ethane, bromo- (8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN Bromic ether
CN Bromoethane
CN Ethyl bromide
CN F 160B1
CN Hydrobromic ether
CN Monobromoethane
CN NSC 8824
FS 3D CONCORD
MF C2 H5 Br
CI COM
LC STN Files: AGRICOLA, ANABSTR, BEILSTEIN*, BIOBUSINESS, BIOSIS, CA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CHEMSAFE, CIN, CSCHEM, CSNB, DETHERM*, DIPPR*, EMBASE, ENCOMPLIT, ENCOMPLIT2, ENCOMPPAT, ENCOMPPAT2, GMELIN*, HODOC*, HSDB*, IFICDB, IFIPAT, IFIUDB, MEDLINE, MRCK*, MSDS-OHS, NIOSHTIC, PDLCOM*, PIRA, PROMT, PS, RTECS*, SPECINFO, SYNTHLINE, TOXCENTER, TULSA, ULIDAT, USPAT2, USPATFULL, VTB
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)
DT.CA CAplus document type: Book; Conference; Dissertation; Journal; Patent; Preprint; Report
RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)
RLD.P Roles for non-specific derivatives from patents: BIOL (Biological study); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)
RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); CMBI (Combinatorial study); FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)
RLD.NP Roles for non-specific derivatives from non-patents: ANST (Analytical study); FORM (Formation, nonpreparative); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

6356 REFERENCES IN FILE CA (1907 TO DATE)
97 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
6358 REFERENCES IN FILE CAPLUS (1907 TO DATE)
6 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L9 ANSWER 45 OF 46 REGISTRY COPYRIGHT 2004 ACS on STN
RN **74-88-4** REGISTRY
CN Methane, iodo- (8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN Iodomethane
CN Methyl iodide
CN Methyl iodide (CH3I)
CN Monoiodomethane
CN NSC 9366
FS 3D CONCORD
DR 147937-07-3
MF C H3 I
CI COM
LC STN Files: AGRICOLA, ANABSTR, BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CHEMSAFE, CIN, CSCHEM, CSNB, DETHERM*, DIPPR*, EMBASE, ENCOMPLIT, ENCOMPLIT2, ENCOMPPAT, ENCOMPPAT2, GMELIN*, HODOC*,

HSDB*, IFICDB, IFIPAT, IFIUDB, MEDLINE, MRCK*, MSDS-OHS, NAPRALERT, NIOSHTIC, PDLCOM*, PIRA, PROMT, PS, RTECS*, SPECINFO, TOXCENTER, TULSA, ULIDAT, USPAT2, USPATFULL, VTB
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)

DT.CA CAplus document type: Book; Conference; Dissertation; Journal; Patent; Preprint; Report

RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study); CMBI (Combinatorial study); FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)

RLD.P Roles for non-specific derivatives from patents: ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)

RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); CMBI (Combinatorial study); FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)

RLD.NP Roles for non-specific derivatives from non-patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

17991 REFERENCES IN FILE CA (1907 TO DATE)
293 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
18016 REFERENCES IN FILE CAPLUS (1907 TO DATE)
13 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L9 ANSWER 46 OF 46 REGISTRY COPYRIGHT 2004 ACS on STN
RN **56-12-2** REGISTRY
CN Butanoic acid, 4-amino- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Butyric acid, 4-amino- (7CI, 8CI)
OTHER NAMES:
CN γ-Aminobutanoic acid
CN γ-Aminobutryic acid
CN γ-Aminobutyric acid
CN ω-Aminobutyric acid
CN 3-Carboxypropylamine
CN 4-Aminobutanoic acid
CN 4-Aminobutyric acid
CN Aminalon
CN GABA
CN Gaballon
CN Gamarex
CN Gammalon
CN Gammalone
CN Gammar
CN Gammasol
CN Mielogen
CN Mielomade
CN NSC 27418
CN NSC 32044
CN NSC 45460
CN NSC 51295
CN Piperidic acid
CN Piperidinic acid
FS 3D CONCORD
DR 3131-86-0
MF C4 H9 N O2
CI COM
LC STN Files: ADISNEWS, AGRICOLA, ANABSTR, BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CABA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, DDFU, DETHERM*, DRUGU, EMBASE, GMELIN*, HODOC*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*, MSDS-OHS, NAPRALERT, NIOSHTIC, PROMT, PS, RTECS*, SPECINFO, SYNTHLINE, TOXCENTER, ULIDAT, USAN, USPAT2, USPATFULL, VETU
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)

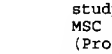
DT.CA CAplus document type: Book; Conference; Dissertation; Journal; Patent; Report

RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study); CMBI (Combinatorial study); FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)

RLD.P Roles for non-specific derivatives from patents: ANST (Analytical study); BIOL (Biological study); CMBI (Combinatorial study); MSC (Miscellaneous); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)

RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); CMBI (Combinatorial study); FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)

RLD.NP Roles for non-specific derivatives from non-patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

26488 REFERENCES IN FILE CA (1907 TO DATE)
453 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
26518 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> D HIS

(FILE 'HOME' ENTERED AT 10:43:22 ON 08 SEP 2004)

FILE 'REGISTRY' ENTERED AT 10:43:34 ON 08 SEP 2004
L1 STRUCTURE UPLOADED
L2 0 S L1
L3 7 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 10:44:26 ON 08 SEP 2004
L4 2 S L3

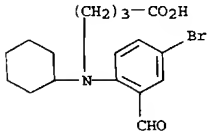
FILE 'REGISTRY' ENTERED AT 10:47:42 ON 08 SEP 2004
L5 STRUCTURE UPLOADED
L6 0 S L5
L7 0 S L5 SSS FULL

FILE 'CAPLUS' ENTERED AT 10:50:41 ON 08 SEP 2004
L8 1 S 2001:185710/AN
SEL RN

FILE 'REGISTRY' ENTERED AT 10:52:01 ON 08 SEP 2004
L9 46 S E1-E46

=> D 3

L9 ANSWER 3 OF 46 REGISTRY COPYRIGHT 2004 ACS on STN
RN **329347-33-3** REGISTRY
CN Butanoic acid, 4-[(4-bromo-2-formylphenyl)cyclohexylamino]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H22 Br N O3
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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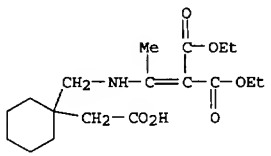
L3 ANSWER 1 OF 7 REGISTRY COPYRIGHT 2004 ACS on STN
RN 478297-17-5 REGISTRY
CN Propanedioic acid, [1-[[[1-(carboxymethyl)cyclohexyl]methyl]amino]ethylidene]-, 1,3-diethyl ester, compd. with piperidine (1:1) (9CI) (CA INDEX NAME)
MF C18 H29 N O6 . C5 H11 N
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)

CM 1

CRN 478297-16-4
CMF C18 H29 N O6



CM 2

CRN 110-89-4
CMF C5 H11 N

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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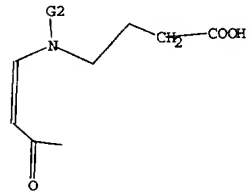
L5 HAS NO ANSWERS
L5 STR



G1 N,P,X,CF2,CF3,CCl2,CCl3,CBr2,CBr3,CI2,CI3,CN,NO2,Cy
G2 C,S

Structure attributes must be viewed using STN Express query preparation.

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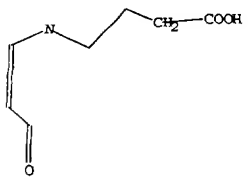
L1 HAS NO ANSWERS
L1 STR



G1 N,P,X,CF2,CF3,CCl2,CCl3,CBr2,CBr3,CI2,CI3,CN,NO2,Cy

G2 C,S

Structure attributes must be viewed using STN Express query preparation.

=> FILE REG

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	94.20	422.49
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-1.40

FILE 'REGISTRY' ENTERED AT 11:05:13 ON 08 SEP 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 7 SEP 2004 HIGHEST RN 741217-26-5
DICTIONARY FILE UPDATES: 7 SEP 2004 HIGHEST RN 741217-26-5

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

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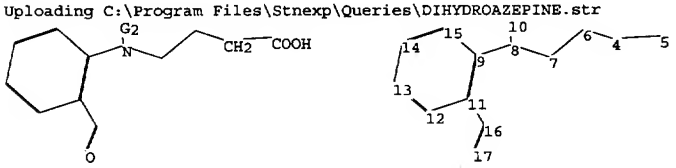


chain nodes :
4 5 10 16 17
ring nodes :
9 11 12 13 14 15
ring/chain nodes :
6 7 8
chain bonds :
4-5 4-6 6-7 7-8 8-9 8-10 11-16 16-17
ring bonds :
9-11 9-15 11-12 12-13 13-14 14-15
exact/norm bonds :
7-8 8-9 8-10 16-17
exact bonds :
4-5 4-6 6-7 11-16
normalized bonds :
9-11 9-15 11-12 12-13 13-14 14-15

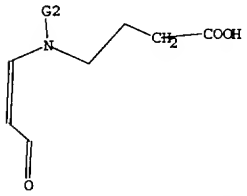
G1:N,P,X,CF2,CF3,CCl2,CCl3,CBr2,CBr3,CI2,CI3,CN,NO2,Cy

G2:C,S

Match level :
4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:CLASS

L10 STRUCTURE UPLOADED

=> D L10
L10 HAS NO ANSWERS
L10 STR



G1 N,P,X,CF2,CF3,CCl2,CCl3,CBr2,CBr3,CI2,CI3,CN,NO2,Cy

G2 C,S

Structure attributes must be viewed using STN Express query preparation.

=> S L10
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SAMPLE SCREEN SEARCH COMPLETED - 405 TO ITERATE

100.0% PROCESSED 405 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:	ONLINE	**COMPLETE**
	BATCH	**COMPLETE**
PROJECTED ITERATIONS:	6893 TO	9307
PROJECTED ANSWERS:	0 TO	0

L11 0 SEA SSS SAM L10

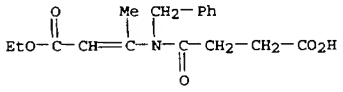
=> S L10 SSS FULL
FULL SEARCH INITIATED 11:05:40 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 8024 TO ITERATE

100.0% PROCESSED 8024 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

L12 1 SEA SSS FUL L10

=> D

L12 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN
RN 115398-14-6 REGISTRY
CN 2-Butenoic acid, 3-[(3-carboxy-1-oxopropyl)(phenylmethyl)amino]-, 1-ethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H21 N O5
SR CA
LC STN Files: CA, CAPLUS, CASREACT
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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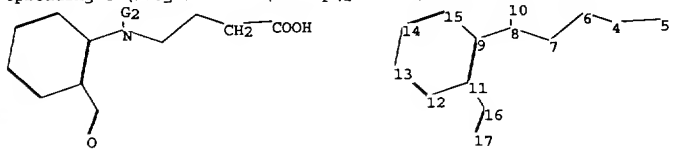


chain nodes :
4 5 10 16 17
ring nodes :
9 11 12 13 14 15
ring/chain nodes :
6 7 8
chain bonds :
4-5 4-6 6-7 7-8 8-9 8-10 11-16 16-17
ring bonds :
9-11 9-15 11-12 12-13 13-14 14-15
exact/norm bonds :
7-8 8-9 8-10 16-17
exact bonds :
4-5 4-6 6-7 11-16
normalized bonds :
9-11 9-15 11-12 12-13 13-14 14-15

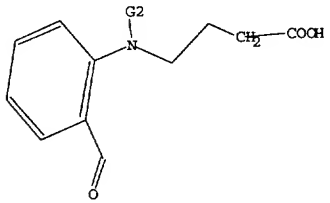
G1:N,P,X,CF2,CF3,CCl2,CCl3,CBr2,CBr3,CI2,CI3,CN,NO2,Cy

G2:C,S

Match level :
4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:CLASS

L13 STRUCTURE UPLOADED

=> D L13
L13 HAS NO ANSWERS
L13 STR



G1 N,P,X,CF2,CF3,CCl2,CCl3,CBr2,CBr3,CI2,CI3,CN,NO2,Cy
G2 C,S

Structure attributes must be viewed using STN Express query preparation.

=> S L13
SAMPLE SEARCH INITIATED 11:08:11 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 11 TO ITERATE

100.0% PROCESSED 11 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 22 TO 418
PROJECTED ANSWERS: 0 TO 0

L14 0 SEA SSS SAM L13

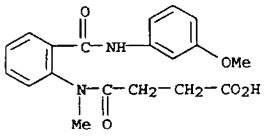
=> S L13 SSS FULL
FULL SEARCH INITIATED 11:08:17 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 159 TO ITERATE

100.0% PROCESSED 159 ITERATIONS 16 ANSWERS
SEARCH TIME: 00.00.01

L15 16 SEA SSS FUL L13

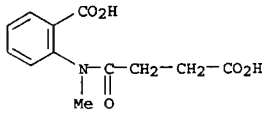
=> D 1-16

L15 ANSWER 1 OF 16 REGISTRY COPYRIGHT 2004 ACS on STN
RN 730976-62-2 REGISTRY
CN Butanoic acid, 4-[[2-[[(3-methoxyphenyl)amino]carbonyl]phenyl]methylamino]-4-oxo- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H20 N2 O5
SR Chemical Library



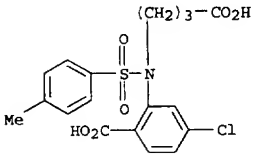
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L15 ANSWER 2 OF 16 REGISTRY COPYRIGHT 2004 ACS on STN
RN 401941-15-9 REGISTRY
CN Benzoic acid, 2-[(3-carboxy-1-oxopropyl)methylamino]- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN NSC 686141
FS 3D CONCORD
MF C12 H13 N O5
SR Chemical Library
LC STN Files: CHEMCATS



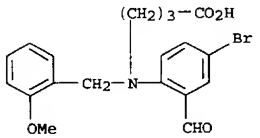
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L15 ANSWER 3 OF 16 REGISTRY COPYRIGHT 2004 ACS on STN
RN 351004-15-4 REGISTRY
CN Benzoic acid, 2-[(3-carboxypropyl)[(4-methylphenyl)sulfonyl]amino]-4-chloro- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H18 Cl N O6 S
SR CAS Client Services



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L15 ANSWER 4 OF 16 REGISTRY COPYRIGHT 2004 ACS on STN
RN 329347-35-5 REGISTRY
CN Butanoic acid, 4-[(4-bromo-2-formylphenyl)[(2-methoxyphenyl)methyl]amino]-(9CI) (CA INDEX NAME)
MF C19 H20 Br N O4
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)



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1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L15 ANSWER 5 OF 16 REGISTRY COPYRIGHT 2004 ACS on STN
RN 329347-34-4 REGISTRY
CN Butanoic acid, 4-[(4-bromo-2-formylphenyl)-2-propenylamino]- (9CI) (CA INDEX NAME)
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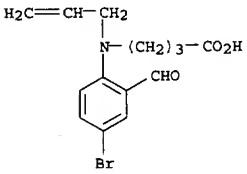
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)



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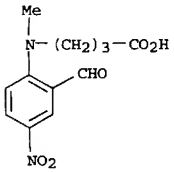
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L15 ANSWER 6 OF 16 REGISTRY COPYRIGHT 2004 ACS on STN
RN 329347-32-2 REGISTRY
CN Butanoic acid, 4-[(2-formyl-4-nitrophenyl)methylamino]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C12 H14 N2 O5
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)



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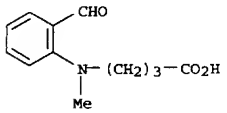
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L15 ANSWER 7 OF 16 REGISTRY COPYRIGHT 2004 ACS on STN
RN 329347-31-1 REGISTRY
CN Butanoic acid, 4-[(2-formylphenyl)methylamino]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C12 H15 N O3
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)



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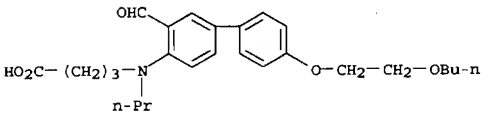
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

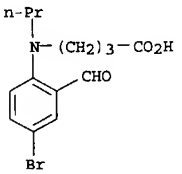
L15 ANSWER 8 OF 16 REGISTRY COPYRIGHT 2004 ACS on STN
RN 329347-29-7 REGISTRY
CN Butanoic acid, 4-[[4'-(2-butoxyethoxy)-3-formyl[1,1'-biphenyl]-4-yl]propylamino]- (9CI) (CA INDEX NAME)
MF C26 H35 N O5
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L15 ANSWER 9 OF 16 REGISTRY COPYRIGHT 2004 ACS on STN
RN 329347-27-5 REGISTRY
CN Butanoic acid, 4-[(4-bromo-2-formylphenyl)propylamino]- (9CI) (CA INDEX NAME)
MF C14 H18 Br N O3
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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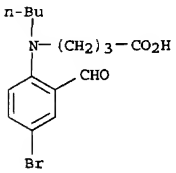
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

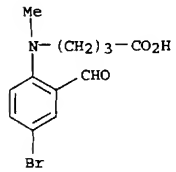
L15 ANSWER 10 OF 16 REGISTRY COPYRIGHT 2004 ACS on STN
RN 329347-25-3 REGISTRY
CN Butanoic acid, 4-[(4-bromo-2-formylphenyl)butylamino]- (9CI) (CA INDEX NAME)
MF C15 H20 Br N O3
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

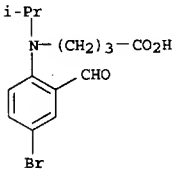
L15 ANSWER 11 OF 16 REGISTRY COPYRIGHT 2004 ACS on STN
RN 329347-22-0 REGISTRY
CN Butanoic acid, 4-[(4-bromo-2-formylphenyl)methylamino]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C12 H14 Br N O3
SR CA
LC STN Files: CA, CAPLUS, CASREACT
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

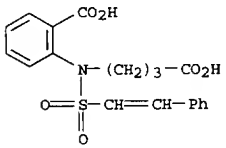
L15 ANSWER 12 OF 16 REGISTRY COPYRIGHT 2004 ACS on STN
RN 313737-28-9 REGISTRY
CN Butanoic acid, 4-[(4-bromo-2-formylphenyl)(1-methylethyl)amino]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C14 H18 Br N O3
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

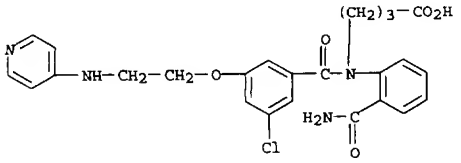
3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L15 ANSWER 13 OF 16 REGISTRY COPYRIGHT 2004 ACS on STN
RN 300375-50-2 REGISTRY
CN Benzoic acid, 2-[(3-carboxypropyl)[(2-phenylethenyl)sulfonyl]amino]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H19 N O6 S
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

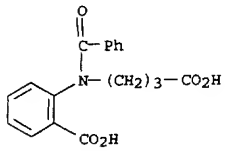
L15 ANSWER 14 OF 16 REGISTRY COPYRIGHT 2004 ACS on STN
RN 192806-33-0 REGISTRY
CN Butanoic acid, 4-[[2-(aminocarbonyl)phenyl][3-chloro-5-[2-(4-pyridinylamino)ethoxy]benzoyl]amino]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C25 H25 Cl N4 O5
SR CA
LC STN Files: CA, CAPLUS, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

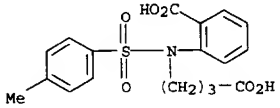
L15 ANSWER 15 OF 16 REGISTRY COPYRIGHT 2004 ACS on STN
RN 107520-71-8 REGISTRY
CN Anthranilic acid, N-benzoyl-N-(3-carboxypropyl)- (6CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H17 N O5
SR CAOLD
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS
(*File contains numerically searchable property data)
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: NORL (No role in record)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L15 ANSWER 16 OF 16 REGISTRY COPYRIGHT 2004 ACS on STN
RN 101730-78-3 REGISTRY
CN Anthranilic acid, N-(3-carboxypropyl)-N-p-tolylsulfonyl- (6CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H19 N O6 S
SR CAOLD
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CHEMCATS
(*File contains numerically searchable property data)
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: NORL (No role in record)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> FILE CAPLUS

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	343.03	765.52
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-1.40

FILE 'CAPLUS' ENTERED AT 11:09:16 ON 08 SEP 2004
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FILE COVERS 1907 - 8 Sep 2004 VOL 141 ISS 11
FILE LAST UPDATED: 7 Sep 2004 (20040907/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> S L14
L16 0 L14

=> S L15
L17 6 L15

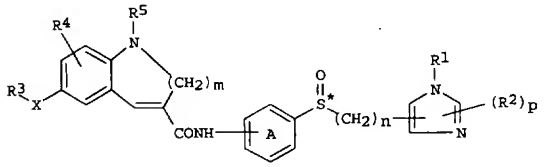
=> D 1-6 IBIB ABS HITSTR

L17 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:737732 CAPLUS
DOCUMENT NUMBER: 139:246034
TITLE: Process for producing optically active imidazolylalkyl acylaminophenyl sulfoxide derivative
INVENTOR(S): Tawada, Hiroyuki; Ikemoto, Tomomi; Nishiguchi, Atsuko; Ito, Tatsuya; Adachi, Mari
PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan

SOURCE: PCT Int. Appl., 103 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003076411	A1	20030918	WO 2003-JP2840	20030311
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
JP 2004123694	A2	20040422	JP 2003-65258	20030311
PRIORITY APPLN. INFO.:			JP 2002-66809 A	20020312
			JP 2002-229802 A	20020807

OTHER SOURCE(S): MARPAT 139:246034
GI



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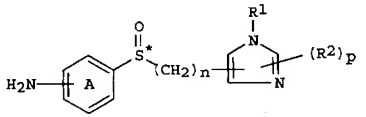

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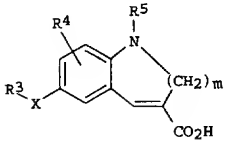


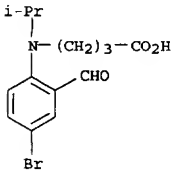
III

AB Disclosed is a process for producing an optically active imidazolylalkyl acylaminophenyl sulfoxide derivative (I) [wherein R1 = (un)substituted aliphatic hydrocarbon or aromatic group; R2 = halo, NO2, cyano, each (un)substituted alkyl, cycloalkyl, HO, NH2, acyl, or aromatic group, CO2H or its ester, (un)substituted SH, sulfinyl, or sulfonyl; the ring A = benzene ring optionally substituted by halo, C1-4 alkyl, C1-4-haloalkyl, C1-4 alkoxy, C1-4 haloalkoxy; n = an integer of 0-3; p = an integer of 0-2; * denotes an asym. center; R3 = 5 or 6-membered ring; R4 = H, halo each (un)substituted lower alkyl or lower alkoxy; R5 = H, each (un)substituted hydrocarbon, aromatic group, sulfonyl, or acyl, CO2H or its ester or amide; X = a bond, a divalent group consisting of 1-4 atoms in the straight chain portion] or a salt thereof, which comprises reacting an imidazolylalkyl aminophenyl sulfoxide derivative (II; R1, R2, the ring A, n, p, * = same as above) with a benzoazacycloalkenecarboxylic acid derivative (III; R3-R5, m, X = same as above) or its salt or reactive derivative This process does not cause side reactions such as racemization and Pummerer rearrangement and is industrially advantageous for the preparation of the title compds. which have CCR5 antagonistic activity (no data). Thus, 27.9 mL Et3N was added dropwise to a solution of 12.5 g 4-aminobenzenethiol in 180 mL THF, followed by adding dropwise 28.2 mL trifluoroacetic anhydride at 0-10°, and the resulting mixture was stirred at 0-5° for 0.5, treated with 30 mL tap water, and stirred at room temperature for 0.5 h to give, after workup and crystallization from n-hexane, 26.1 g 2,2,2-trifluoro-N-(4-mercaptophenyl)acetamide (IV). Et3N (29.0 mL) was added to a solution of 24.8 g IV in 99 mL MeOH, followed by adding a solution of 20.4 g 5-(chloromethyl)-1-propyl-1H-imidazole hydrochloride in 21 mL H2O at 0-20°, and the resulting mixture was stirred at 20-30° for 0.5 h to give after workup and crystallization from iso-Pr ether, 73% 2,2,2-trifluoro-N-[4-[[(1-propyl-1H-imidazol-5-yl)methyl]thio]phenyl]acetamide (V). 30% Aqueous H2O2 (16.4 g) was added to a solution of 33.1 g V in 49.7 mL at 2-30°, stirred at the same temperature for 3 h and treated with 330 mL EtOAc, followed by adding 35.9 g Na2S2O3.5 H2O at 0-10° and then dropwise 144.6 mL 6 N aqueous NaOH, and the resulting mixture was stirred at the same temperature for 0.5 h to give, after workup, 2,2,2-trifluoro-N-[4-[[(1-propyl-1H-imidazol-5-yl)methyl]sulfinyl]phenyl]acetamide which was dissolved in 198.6 mL MeOH, treated with a solution of 40.0 g K2CO3 in 99.3 mL H2O and stirred at 50° for 2.5 h to give, after workup including decolorization with activated charcoal and crystallization from EtOAc, 73% 4-[[(1-propyl-1H-imidazol-5-yl)methyl]sulfinyl]phenylamine (VI). H2O (90 mL) was added dropwsie to a solution of 15.1 g di-p-toluoyl-D-tartaric acid (VII) and 10.3 g VI in 1,2-dimethoxyethane and stirred at room temperature overnight, followed by filtration of the precipitated crystals, washing with 50% by volume aqueous 1,2-dimethoxyethane (30 mL), vacuum-drying, recrystn. from aqueous MeCN, and vacuum-drying to give, 41.6% (-)-VI.VII diastereomer salt (99.6% de). (-)-VI.VII diastereomer salt (5 g) was extracted with 3 N aqueous HCl and 20 mL EtOAc and the aqueous layer was treated with 5 mL EtOAc 6 N aqueous NaOH to adjust pH at .apprx.9, seeded with crystals, stirred at room temperature, and filtered to give 95.4% (-)-VI (1.88 g) as a white powder. A solution of 2.56 g 7-[4-(2-butoxyethoxy)phenyl]-1-isobutyl-2,3-dihydro-1H-1-benzazepine-4-carboxylic acid in 7.5 mL THF was treated with one drop of DMF and then dropwise with 0.56 mL oxalyl chloride at room temperature, and stirred for 1 h to give a solution of the acid chloride which was added dropwsie to a solution of (-)-VI, similarly prepared from 5 g (-)-VI.VII diastereomer salt, in 17.5 mL THF and 2.85 mL Et3N at room temperature and stirred at room temperature for 1 h to give, after workup including treatment with silica gel and activated charcoal, and crystallization from ethanol-tert-Bu Me ether, 78% (-)-7-[4-(2-butoxyethoxy)phenyl]-1-isobutyl-N-[4-[[(1-propyl-1H-imidazol-5-yl)methyl]sulfinyl]phenyl]-2,3-dihydro-1H-1-benzazepine-4-carboxamide.

IT **313737-28-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of optically active imidazolylalkyl acylaminophenyl sulfoxide derivs. by amidation of optically active imidazolylalkyl aminophenyl sulfoxides with benzoazacycloalkenecarboxylic acids as CCR5 antagonists)

RN 313737-28-9 CAPLUS

CN Butanoic acid, 4-[(4-bromo-2-formylphenyl)(1-methylethyl)amino]- (9CI) (CA INDEX NAME)

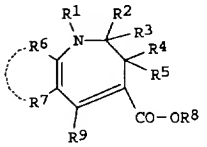


REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:185710 CAPLUS
DOCUMENT NUMBER: 134:222638
TITLE: Process for the preparation of 2,3-dihydroazepine compounds
INVENTOR(S): Ikemoto, Tomomi; Ito, Tatsuya; Nishiguchi, Atsuko; Tomimatsu, Kiminori
PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan
SOURCE: PCT Int. Appl., 59 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001017947	A1	20010315	WO 2000-JP6012	20000905
W: AE, AG, AL, AM, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CN, CR, CU, CZ, DM, DZ, EE, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LV, MA, MD, MG, MK, MN, MX, MZ, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 2000068706	A5	20010410	AU 2000-68706	20000905
EP 1211239	A1	20020605	EP 2000-956925	20000905
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
JP 2001151741	A2	20010605	JP 2000-275003	20000906
PRIORITY APPLN. INFO.:			JP 1999-252334 A	19990906
			WO 2000-JP6012 W	20000905

OTHER SOURCE(S): CASREACT 134:222638; MARPAT 134:222638
GI



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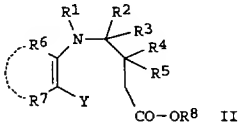
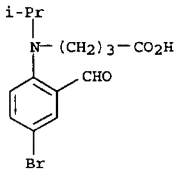


II

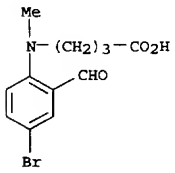
AB 2,3-Dihydroazepine compds. I [R1 = (un)substituted hydrocarbon, etc.; R2 - R7 = H, halo, etc.; further details on R1 - R7 are given; R8 = (un)substituted hydrocarbon; R9 = H, (un)substituted hydrocarbon], useful as intermediates for CCR5 antagonists, are prepared by cyclization of esters II [R1 - R8 = as defined above; Y = COR9; R9 = as defined above]. Intermediates for the preparation of II are also disclosed in this document. Thus, a mixture of Et 4-(4-bromo-2-formyl-N-methylanilino)butyrate, sodium ethoxide solution in ethanol, and di-Et carbonate was stirred at room temperature for 4 h to give, after workup, 7-bromo-1-methyl-2,3-dihydro-1-benzazepine-4-carboxylic acid Et ester in 90% yield.

IT **313737-28-9P 329347-22-0P 329347-25-3P**
329347-27-5P 329347-29-7P 329347-31-1P
329347-32-2P 329347-34-4P 329347-35-5P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(process for preparation of 2,3-dihydroazepine compds.)

RN 313737-28-9 CAPLUS
CN Butanoic acid, 4-[(4-bromo-2-formylphenyl)(1-methylethyl)amino]- (9CI) (CA INDEX NAME)

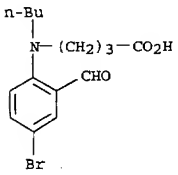


RN 329347-22-0 CAPLUS
CN Butanoic acid, 4-[(4-bromo-2-formylphenyl)methylamino]- (9CI) (CA INDEX NAME)

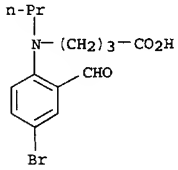


RN 329347-25-3 CAPLUS
CN Butanoic acid, 4-[(4-bromo-2-formylphenyl)butylamino]- (9CI) (CA INDEX

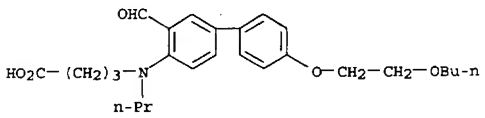
NAME)



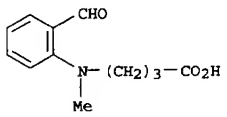
RN 329347-27-5 CAPLUS
CN Butanoic acid, 4-[(4-bromo-2-formylphenyl)propylamino]- (9CI) (CA INDEX NAME)



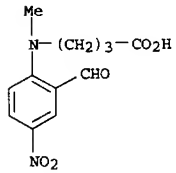
RN 329347-29-7 CAPLUS
CN Butanoic acid, 4-[[4'-(2-butoxyethoxy)-3-formyl[1,1'-biphenyl]-4-yl]propylamino]- (9CI) (CA INDEX NAME)



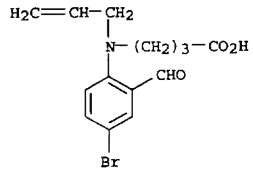
RN 329347-31-1 CAPLUS
CN Butanoic acid, 4-[(2-formylphenyl)methylamino]- (9CI) (CA INDEX NAME)



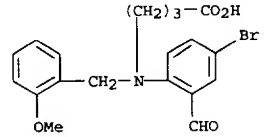
RN 329347-32-2 CAPLUS
CN Butanoic acid, 4-[(2-formyl-4-nitrophenyl)methylamino]- (9CI) (CA INDEX NAME)



RN 329347-34-4 CAPLUS
CN Butanoic acid, 4-[(4-bromo-2-formylphenyl)-2-propenylamino]- (9CI) (CA INDEX NAME)



RN 329347-35-5 CAPLUS
CN Butanoic acid, 4-[(4-bromo-2-formylphenyl)[(2-methoxyphenyl)methyl]amino]- (9CI) (CA INDEX NAME)



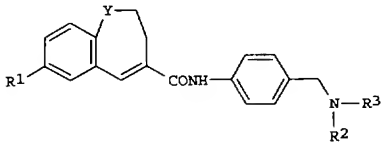
REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:900630 CAPLUS
DOCUMENT NUMBER: 134:56698
TITLE: Preparation process and effect of benzazepine derivatives as CCR5 antagonists
INVENTOR(S): Shiraishi, Mitsuru; Baba, Masanori; Aramaki, Yoshio; Kanzaki, Naoyuki; Nishimura, Osamu
PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan
SOURCE: PCT Int. Appl., 342 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

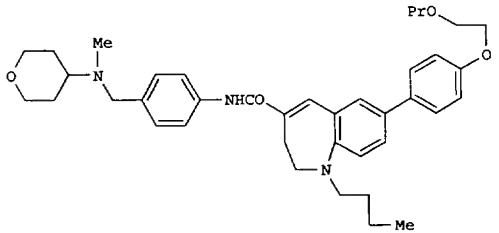
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

WO 2000076993	A1	20001221	WO 2000-JP3879		20000615
W: AE, AG, AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CR, CU, CZ, DM, DZ, EE, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LV, MA, MD, MG, MK, MN, MX, MZ, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
EP 1186604	A1	20020313	EP 2000-939065		20000615
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO					
JP 2001058992	A2	20010306	JP 2000-185904		20000616
PRIORITY APPLN. INFO.:			JP 1999-170345	A	19990616
			WO 2000-JP3879	W	20000615

OTHER SOURCE(S): MARPAT 134:56698
GI



I

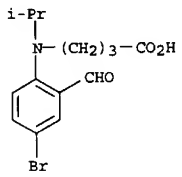


II

AB Title compds. [I; R1 is a five- or six-membered aromatic ring which bears a substituent represented by the general formula: RZ1XZ2; R is hydrogen or optionally substituted hydrocarbyl; X is optionally substituted alkylene; and Z1 and Z2 are each a heteroatom and may be further substituted, with R being optionally bonded to the aromatic ring to form another ring; Y is optionally substituted imino; and R2 and R3 are each optionally substituted aliphatic hydrocarbyl or an optionally substituted hetero-alicyclic group] and salts, which exhibit CCR5 antagonism and exert preventive and therapeutic effects against HIV infections in mammal. Thus, the title compound II was prepared

IT **313737-28-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation process and effect of benzazepine derivs. as CCR5 antagonists)

RN 313737-28-9 CAPLUS
CN Butanoic acid, 4-[(4-bromo-2-formylphenyl)(1-methylethyl)amino]- (9CI) (CA INDEX NAME)

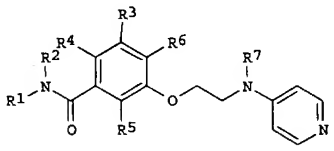


REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1997:503143 CAPLUS
DOCUMENT NUMBER: 127:121643
TITLE: Preparation of 5-[2-(pyridin-4-ylamino)ethoxy]benzamides as thrombin inhibitors
INVENTOR(S): Watson, Nigel Stephen; Pass, Martin; Patel, Vipulkumar
PATENT ASSIGNEE(S): Glaxo Group Limited, UK; Watson, Nigel Stephen; Pass, Martin; Patel, Vipulkumar
SOURCE: PCT Int. Appl., 139 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 9722589	A1	19970626	WO 1996-EP5743		19961213
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG					
AU 9713030	A1	19970714	AU 1997-13030		19961213
JP 2000503634	T2	20000328	JP 1997-522517		19961213
EP 1021411	A1	20000726	EP 1996-944604		19961213
EP 1021411	B1	20030305			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO					
AT 233733	E	20030315	AT 1996-944604		19961213
ES 2196197	T3	20031216	ES 1996-944604		19961213
US 6326386	B1	20011204	US 2000-678610		20001004
PRIORITY APPLN. INFO.:			GB 1995-25620	A	19951215
			WO 1996-EP5743	W	19961213
			US 1998-77885	B1	19980612

OTHER SOURCE(S): MARPAT 127:121643
GI



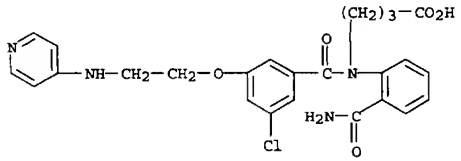
I

AB The title compds. [I; R1, R2 = XR8 (wherein X = a bond, C1-6 alkylene, C3-6 alkenylene, etc.; R8 = H, C3-7 cycloalkyl, aryl, etc.); R1R2 = (un)substituted C3-7 heterocycloalkyl, heterocycloalkenyl; R3 = H, C1-3 alkyl, halo, C1-2 alkoxy; R4-R6 = H, halo; R7 = H, C1-6 alkyl] and their salts, useful as thrombin inhibitors, were prepared and formulated. Thus, reaction of 3-methyl-5-[2-(pyridin-4-ylamino)ethoxy]benzoic acid.CF3COOH with N-methylcyclohexylamine in the presence of HOBt, TBTU and DIPEA in DMF afforded I.CF3COOH [R1 = Me; R2 = cyclohexyl; R3 = Me; R4-R7 = H] which showed IC50 of 8 nM.

IT **192806-33-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 5-[2-(pyridin-4-ylamino)ethoxy]benzamides as thrombin inhibitors)

RN 192806-33-0 CAPLUS

CN Butanoic acid, 4-[[2-(aminocarbonyl)phenyl][3-chloro-5-[2-(4-pyridinylamino)ethoxy]benzoyl]amino]- (9CI) (CA INDEX NAME)



L17 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1959:29140 CAPLUS
DOCUMENT NUMBER: 53:29140
ORIGINAL REFERENCE NO.: 53:5283c-i,5284a-g
TITLE: Structure and properties of certain polycyclic indolo and quinolino derivatives. XI. Derivatives of 4,5,6,7-tetrahydro-1-methyl-4-oxo-2,3-benzazepine
AUTHOR(S): Braunholtz, John T.; Mann, Frederick G.
CORPORATE SOURCE: Univ. Chem. Lab., Cambridge, UK
SOURCE: Journal of the Chemical Society, Abstracts (1958) 3377-86
CODEN: JCSAAZ; ISSN: 0590-9791
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 53:29140

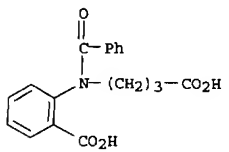
AB 4,5,6,7-Tetrahydro-1-methyl-4-oxo2,3-benzazepine (I) in its simple reactions resembles 1,2,3,4-tetrahydro-1-methyl-4-oxoquinoline (II), but its indolo (III) and quinolino derivs. (IV) differ markedly from those of II. The Fischer reaction with I phenylhydrazone (V) yields a true indole instead of a ψ-indole. The quinolino acid (VI) obtained by the Pfitzinger reaction does not show the marked resonance and deep color of the oxoquinoline derivative, and the corresponding base IV, obtained by decarboxylation of the acid or by direct application of the Friedlander reaction, does not undergo acid-catalyzed allylic rearrangement or ready oxidation to a cyclic amide. Dry HBr bubbled into absolute alc. at 0° until 100 g. absorbed, 67 g. γ-butyrolactone added, the mixture refluxed 4.5 hrs., and fractionally distilled gave 100 g. crude Br(CH2)3CO2Et (VIII), b14 85-7°, n20D 1.451. Attempts to prepare the Me ester by analogous procedure were unsuccessful. VIII (100 g.) and 200 g. Me anthranilate (IX) heated 12 hrs. at 100°, the pasty crystalline mass shaken with 400 cc. H2O to which excess NaHCO3 was gradually added, the mixture extracted with Et2O, dried, and distilled gave 150 g. unchanged IX, b0.4 115-20°, and 75 g. Me N-(3-ethoxycarbonylpropyl)anthranilate (X), b0.07 176-80°, m. 43.5° (ligroine). X (5 g.) in 25 cc. aqueous alc. containing 7 g. KOH refluxed 1 hr., cooled, and acidified to pH 6 gave 3.9 g. diacid (XI), m. 190° (effervescence) (alc.). X (5 g.) in 20 cc. C5H5N treated gradually with 4.2. g. BzCl, heated 1 hr. at 50°, cooled, poured into 300 cc. H2O, the oil collected, washed, and fractionally distilled gave an almost quant. yield of Me N-benzoyl-N-(3-ethoxycarbonylpropyl)anthranilate (XII), b0.05 215-25°, m. 46° (Et2O-ligroine). XII (1 g.) was quant. hydrolyzed by refluxing 45 min. in 50% aqueous alc. containing 2 g. KOH and acidifying to give N-benzoyl-N-(3-carboxypropyl)anthranilic acid (XIII), m. 175° (aqueous alc.). Unsuccessful attempts to form the 7-membered ring of the benzazepine system were made. (a) XI treated with Ac2O and KOAc under a variety of conditions. (b) XII in xylene refluxed 9 hrs. with Na gave no ketonic product. X (30 g.) and 45 g. MeI heated 4 hrs. at 90° in an autoclave, the cold product added to 100 cc. H2O and 50 cc. Et2O and treated with excess NaHCO3, the mixture extracted with Et2O, dried, and evaporated gave 18 g. Me N-(3-ethoxycarbonylpropyl)-N-methylanthranilate (XIV), b0.03 139°. In a typical Dieckmann cyclization a solution of 6 g. XIV in 35 cc. xylene added during 45 min. to a suspension of 1 g. Na in 120 cc. refluxing xylene under N, the refluxing continued 7-12 hrs., the excess Na decomposed, the xylene solution extracted with 6N HCl, the aqueous extract refluxed 45 min. in N, cooled, treated with NaHCO3, extracted with Et2O, and fractionally distilled gave 1.8 g. I, b0.2 112° which did not crystalline; it was stable for several weeks under normal conditions. When the above procedure was repeated using PhMe to replace xylene a yield of 42% I was obtained; using 1 g. atom Na in xylene containing a trace of MeOH and refluxing 10 hrs. the yield was 42%. The Dieckmann reaction with Na in anhydrous C6H6 containing a trace of MeOH gave 27% yield, and the use of NaH in dry C6H6 gave only traces of ketonic material. I (0.5 g.) in 5 cc. alc. containing 2 cc. H2O treated under reflux 2 hrs. with 0.35 H2NCONHNH2.HCl and NaOAc gave 0.5 g. I semicarbazone, m. 198° (alc.); 2,4-dinitrophenylhydrazone, m. 202-3°; V, viscous sirup which did not crystalline; HCl salt, m. 160-1° (decomposition) (alc.); picrate, not pure. All attempts to isolate crystalline products of condensation between the 5-CH2 group of I and p-Me2NC6H4CHO or p-ONC6H4NMe2 failed; the former reagent gave no reaction, and the latter gave intractable tars. V (from 1.4 g. I) refluxed 8 hrs. in a mixture of saturated alc. HCl and alc., cooled 2 hrs. at 0°, and the product collected gave 2.1 g. 6,7-dihydro-1-methyl-2,3-benzindolo[2,'3'4,5]azepine-HCl (XV), m. 235° (effervescence). An aqueous alc. solution of XV basified with 10% aqueous NaOH gave the free indolo compound (III), m. 119° (aqueous alc.). III is completely stable when exposed to air; a slow and partial oxidation occurs in hot Me2COKMnO4, but no pure derivative was isolated. III shows infrared absorption maximum at 3420 and 3380 and a shoulder at 2800 cm.-1 The similarity between the ultraviolet spectra of III in alc. and in alc. HCl accords with the protonation of the benzazepine-N atom rather than that of a ψ-indole. Unsuccessful attempts were also made to dehydrogenate III at the saturated 6,7-linkage, by reagents such as Pd-C or chloranil. Isatin (1.4 g.) and 1.7 g. KOH in 5 cc. H2O refluxed 10 hrs. with 1.4 g. I in 10 cc. alc. gave

0.75 g. 6,7-dihydro-1-methyl-2,3-benzoquinolino [2',3'4,5] azepine-4'-carboxylic acid (VI), m. 295° (slow effervescence). I (0.7 g.) in 10 cc. warm alc. treated with 0.5 g. o-H2NC6H4CHO and left at room temperature 1 week under N gave 0.8 g. 6,7-dihydro-1-methyl-2,3-benzoquinolino[2',3'-4,5]azepine (IV), m. 127° (aqueous alc.). IV distils smoothly in the sublimation tube at 300°/15 mm. without change. VI heated in a tube at 0.002 mm. sublimed at 250-310° without residue. The yellow crystalline sublimate was identical with unchanged VI. In a similar experiment at 15 mm. a clear viscous orange distillate was obtained at 300°. This product was shown by infrared and chromatographic analysis to be almost pure IV contaminated with traces of VI. IV formed an unstable MeI salt, m. 210-11° (effervescence) (Me2CO containing a trace of MeOH); HCl salt, m. 194-6°; di-HCl salt, m. 200-5° (deep red melt). Attempts to effect the acid-catalyzed isomerization of IV gave the unchanged base or its HCl salt almost quant. after refluxing in dilute HCl for 4 hrs., or in concentrated HCl containing a small amount of dioxane. Identification was confirmed by infrared spectroscopy. IV (50 mg.) in 10 cc. Me2CO treated during 2 hrs. with an excess of saturated Me2CO-KMnO4, the solution refluxed until the color disappeared, cooled, filtered, the filtrate concentrated, filtered again, and cooled gave 50 mg. 6,7-dihydro - 1 - methyl - 7 - oxo - 2,3 - benzoquinolino [2',3' - 4,5]-azepine (XVI), m. 192-3° (aqueous alc.). XVI cannot be obtained at room temperature by atmospheric oxidation in C6H6 or by KMnO4 oxidation in Me2CO, does not form a stable HCl salt and does not react with 2,4-dinitrophenylhydrazine. The disappearance of the N-Me infrared absorption band, the lack of ketonic properties, and the very low basic strength show that this oxidation product is the 7-oxo and not the 6-oxo isomer, which should be ketonic and should absorb in the 2800 cm.-1 region. Infrared absorption due to the CO group occurs at 1660 cm.-1 The marked differences between the derivs. of I and II brought about solely by the insertion of one addnl. CH2 group into the oxo amine ring of II, are particularly interesting in connection with the structural features required to facilitate the allylic transformation.

IT **107520-71-8**, Anthranilic acid, N-benzoyl-N-(3-carboxypropyl)- (preparation of)

RN 107520-71-8 CAPLUS

CN Anthranilic acid, N-benzoyl-N-(3-carboxypropyl)- (6CI) (CA INDEX NAME)



L17 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1957:81531 CAPLUS

DOCUMENT NUMBER: 51:81531

ORIGINAL REFERENCE NO.: 51:14756h-i,14757a-e

TITLE: Azabenzocycloheptenones. II. Dieckmann cyclization of arylamino esters

AUTHOR(S): Proctor, G. R.; Thomson, R. H.

CORPORATE SOURCE: Univ. Aberdeen, UK

SOURCE: Journal of the Chemical Society, Abstracts (1957) 2312-14
CODEN: JCSAAZ; ISSN: 0590-9791

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

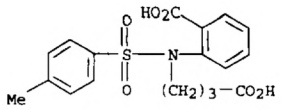
OTHER SOURCE(S): CASREACT 51:81531

AB Attempted acyloin reduction of Me N-(2-methoxycarbonylethyl)anthranilate (I) gave 1,2,3,4-tetrahydro-3-methoxycarbonyl-4-quinolone (II). Dieckmann cyclization of Et γ-N-(2-methoxycarbonylphenyl)-N-p-toluenesulfonamidobutyrate (III) gave 3-p-toluenesulfonyl-3-azabenzocyclohepten-7-one (IV). Anthranilic acid (137 g.) refluxed 18 hrs. with 53 g. acrylonitrile, 20 ml. 40% KOH, and 50 ml. alc. gave 127 g. N-(2-cyanoethyl)anthranilic acid (V), needles, m. 169° (from alc.-H2O). V (40 g.) refluxed with 20% KOH until NH3 ceased to evolve gave 95% N-(2-carboxyethyl)anthranilic acid (VI), m. 182° (from H2O); N-p-toluenesulfonyl derivative, needles, m. 188-9°. VI (46 g.) in 500 ml. MeOH refluxed with passage of HCl, after 12 hrs. the mixture cooled to 0°, and poured into 20% NaOH gave 26.5 g. I, prisms, m. 36° (from ligroine), and 12 g. unchanged VI. In one experiment when passage of HCl was for 50 min. gave N-(2-methoxycarbonylethyl)anthranilic acid, needles, m. 101° (from ligroine). I gave a monoester monoamide, needles, m. 105° (from ligroine). V (230 g.) heated 43 hrs. with 208 g. MeOH and 136 ml. concentrated H2SO4 and the residue distilled at 180-90°/10 mm. Redistn. gave I as the principal fraction and the remainder fractionated at 83°/0.05 g. hydrolyzed gave 2-amino-3-methylbenzoic acid, m. 163.5° (from ligroine); HCl salt, needles, m. 175.5°; Me ester, b0.05 83°, was diazotized and coupled with β-naphthol gave an azo derivative, needles, m. 179°. I (9.25 g.) refluxed 22 hrs. in 75 ml. C6H6 containing 1.2 g. finely dispersed Na and 0.5 g. alc. and the product sublimed in vacuo gave 0.47 g. II, crystals, m. 113°; 2,4-dinitrophenylhydrazone, red needles, m. 221° (from EtOAc-ligroine); O,N-di-p-toluenesulfonyl derivative, needles, m. 136-7°. The residue after sublimation was an oil which gave 1,2,3,4-tetrahydro-4-quinolone 2,4-dinitrophenylhydrazone (VII), m. 260°. Hydrochloric acid hydrolysis of II also gave an oil which formed a 2,4-dinitrophenylhydrazone, m. 260°. I (10 g.) in 400 ml. xylene and added during 8.5 hrs. to a refluxing suspension of 5 g. Na in 200 ml. xylene, and the product distilled at 145°/0.05 mm. and identified as VII. The solid residue was sublimed to give 4.2 g. II. Me anthranilate (50 g.) with 80 g. p-tosyl chloride in 160 ml. C5H5N gave 92 g. Me N-p-toluenesulfonylanthranilate (VIII), prisms, m. 113° (from MeOH). VIII (75 g.), 48 g. Br(CH2)3CO2Et, 90 g. K2CO3, and 200 ml. Me2CO refluxed 24 hrs. gave 89 g. III, needles, m. 102-3° (from EtOAc-ligroine). Alkaline hydrolysis of III gave a diacid, needles, m. 229-31° (from aqueous alc.). K (2 g.) dispersed in 200 ml. C6H6 while hot and 5.5 ml. tert-BuOH added, then during 2 hrs. a solution of 20 g. III in 200 ml. C6H6 added with passage of N, the mixture refluxed a further 20 hrs. and the residue refluxed 1.5 hrs. with 90 ml. alc. and 50 ml. concentrated HCl giving an oil. This oil was purified by refluxing 0.5 hr. with aqueous NaOH or via its 2,4-dinitrophenylhydrazone (IX). IX (4 g.), 1.22 g. m-O2NC6H4CHO, 100 ml. BuOH, and 2 ml. concentrated HCl refluxed 40 hrs. gave IV, needles, m. 126°. Alkaline hydrolysis gave 1.82 g. IV. IX obtained as needles, m. 236°. IV p-nitrobenzylidene derivative formed needles, m. 249-50° (from AcOH).

IT **101730-78-3**, Anthranilic acid, N-(3-carboxypropyl)-N-p-tolylsulfonyl- (preparation of)

RN 101730-78-3 CAPLUS

CN Anthranilic acid, N-(3-carboxypropyl)-N-p-tolylsulfonyl- (6CI) (CA INDEX NAME)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O
S
O
N
Me
(CH2)3—CO2H

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